Analysis of the second order exchange self energy of a dense electron gas

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Abstract

We investigate the evaluation of the six-fold integral representation for the second order exchange contribution to the self energy of a dense three dimensional gas on the Fermi surface.

PACS 71.10.CA, 05.30.Fk

Introduction

The second order exchange energy, represented by the diagram in Fig.1a contributes importantly to the correlation energy of a dense electron gas [1]. It is given by the nine-fold integral

$$E_{2x} = \frac{3}{32\pi^4}\int d^3p_1\int d^3p_2\int \frac{dq^3}{q^2}\frac{f_{p_1}f_{p_2}f'_{p_1+q}f'_{p_2+q}}{(\vec{q}+\vec{p}_1+\vec{p}_2)^2(q^2+p_1\cdot\vec{q}+\vec{p}_2\cdot\vec{q})} \tag{1}$$

in three dimensions, where f_p denotes the Fermi distribution function for electrons of wave vector $\vec{p}$ and f'_p denotes that for holes. In a remarkable display of mathematical virtuosity (1) was evaluated in closed form by Onsager[2] and Onsager, Mittag and Stephen[3] who found

$$E_{2x} = \frac{1}{6}\ln(2) - \frac{3}{4\pi^2}\zeta(3). \tag{2}$$

Subsequently, Ishihara and Ioratti[4] worked out the corresponding value for a two-dimensional system, and the d-dimensional case was evaluated by Glasser[5].

Recently the the second order exchange term in the electron self energy, represented by the diagram in Fig.1b was studied by Ziesche[6]. It is given, in three dimensions, by the six-fold integral

$$\Sigma_{2x}(k) = \frac{1}{4\pi^4}\int\frac{d^3q}{q^2}\int d^3p\frac{f_pf_{k+q}f_{p+q}f'_pf'_{p+q}}{(\vec{k}+\vec{p}+\vec{q})^2(q^2+\vec{k}\cdot\vec{q}+\vec{p}\cdot\vec{q})}. \tag{3}$$

For $k = k_F(=1)$ Ziesche succeeded in decomposing (3) into the sum $\Sigma_{2x} = -(X_1+X_2)/4\pi^2$ of the two simpler integrals

$$X_1 = \int\frac{d^3q_1}{q_1^2}\int\frac{d^3q_2}{q_2^2}\frac{f_{k+q_1+q_2}f'_{k+q_1}f'_{k+q_2}}{\vec{q}_1\cdot\vec{q}_2}$$

$$X_2 = -\int\frac{d^3q_1}{q_1^2}\int\frac{d^3q_2}{q_2^2}\frac{f'_{k+q_1+q_2}f_{k+q_1}f_{k+q_2}}{\vec{q}_1\cdot\vec{q}_2} \tag{4}$$

and by following the procedure in [3], he managed to perform three of the integrations, thereby obtaining

$$X_1 = -16\pi\int_0^1 dp\int_0^1 dq\int_{-1}^1\frac{dx}{(1-p^2q^2)}\frac{F[p,q,x]}{1+q^2}$$

$$X_2 = 16\pi\int_0^1 dp\int_0^1 dq\int_{-1}^1\frac{dx}{(1-p^2q^2)}\frac{q^2F[p,q,x]}{1+q^2} \tag{5}$$

where

$$\alpha = \frac{1-q^2}{2q}, \qquad \beta = \frac{1-p^2}{2p}, \qquad a = \frac{1+p^2q^2}{2pq}$$

$$F[p,q,x] = \frac{2}{a^2-x^2}\tan^{-1}\left[\frac{\alpha x+\beta}{\sqrt{(1+\alpha^2)(1-x^2)}}\right]. \tag{6}$$

The integrals in (6) are suitable for numerical evaluation and Ziesche found $X_1 = -30.70598\ldots$,$X_2 = 21.28490\ldots$.

According to the Hugenholtz-van Hove- Luttinger-Ward theorem[7] $\Sigma_{2x} = E_{2x}$, so

$$X_1 + X_2 = 3\zeta(3) - \frac{2\pi^2}{3}\ln(2). \tag{7}$$

The aim of this note is to evaluate $X = X_2 - X_1$ analytically, so as to obtain closed form expressions for the integrals in (4).

Calculation

From (5) we have

$$X = 16\pi \int_0^1 dq \int_0^1 dp \int_{-1}^1 dx \frac{F[p,q,x]}{1-p^2q^2}. \tag{8}$$

Since the limits on the x-integral are symmetric, we retain only the even part of the integrand of (8) by averaging X and the integral obtained by $x \to -x$ and combining the two arctangents, thus obtaining

$$X = 16\pi \int_0^1 dp \int_0^1 dq \int_0^1 dx \frac{\tan^{-1}\left[\frac{2\beta\sqrt{(1+\alpha^2)(1-x^2)}}{\alpha^2-\beta^2+1-x^2}\right]}{(1-p^2q^2)(a^2-x^2)}. \tag{9}$$

Next, we set $q = e^{-u}$, $p = e^{-v}$, $x = \sin\phi$, so $\alpha = \sinh\ u$, $\beta = \sinh\ v$, $a = \cosh(u+v)$, and

$$X = 8\pi \int_0^\infty du \int_0^\infty dv \int_0^{\pi/2} d\phi\ \cos\ \phi \frac{tan^{-1}\left[\frac{(\sinh(u+v)+\sinh(v-u))\cos\ \phi}{\sinh(u+v)\sinh(u-v)+\cos^2\phi}\right]}{\sinh(u+v)[\sinh^2(u+v)+\cos^2\phi]}. \tag{10}$$

We make the coordinate transformation $r = v+u$, $s = v-u$, having Jacobian 1/2, to obtain

$$X = 4\pi \int_0^\infty dr \int_{-r}^r ds \int_0^{\pi/2} d\phi\ \cos\phi \frac{\tan^{-1}\left[\frac{(\sinh\ r+\sinh\ s)\cos\ \phi}{\cos^2\phi-\sinh\ r\sinh\ s}\right]}{\sinh\ r(\sinh^2 r+\cos^2\phi)}. \tag{11}$$

Since

$$\tan^{-1}\left[\frac{\cos\ \phi(\sinh\ r+\sinh\ s)}{\cos^2\phi - \sinh\ r\sinh\ s}\right] =$$

$$Im\ \ln[(\cos\ \phi + i\sinh\ r)(\cos\ \phi + i\sinh\ s)] =$$

$$\tan^{-1}\left(\frac{\sinh\ r}{\cos\ \phi}\right) + \tan^{-1}\left(\frac{\sinh\ s}{\cos\ \phi}\right), \tag{12}$$

(11) becomes

$$X =$$

$$4\pi \int_0^\infty dr \int_{-r}^{r} ds \int_0^{\pi/2} d\phi \ \cos\ \phi \frac{\tan^{-1}(\sec\ \phi \sinh\ r) + \tan^{-1}(\sec\ \phi \sinh\ s)}{\sinh\ r(\cos^2\phi + \sinh^2 r)} \tag{13}$$

Once again, we may drop the term in the integrand of (13) odd in s and perform the elementary $s-$ integration, so that

$$X = 8\pi \int_0^\infty \frac{rdr}{\sinh\ r} \int_0^{\pi/2} d\phi\ \tan^{-1}\left(\frac{\sinh\ r}{\cos\ \phi}\right) \frac{\cos\ \phi}{\cos^2\phi + \sinh^2 r}. \tag{14}$$

To evaluate the $\phi-$integral, we set $\tan\ \psi = \sec\ \phi \sinh\ r$, $\mu = \tan^{-1}(\sinh\ r) = \cos^{-1}(sech\ r)$, to transform (14) into

$$X = 8\pi \int_0^\infty \frac{rdr}{\sinh\ r} \cos\ \mu \int_\mu^{\pi/2} \frac{\psi \cos\ \psi\ d\psi}{\sqrt{\sin^2\psi - \sin^2\mu}}. \tag{15}$$

The $\psi-$ integral is tabulated[8] and X is reduced to a single integral

$$X = 4\pi^2 \int_0^\infty \frac{r\ sech\ r \ln(1 + sech\ r)}{\sinh\ r} dr. \tag{16}$$

To evaluate the remaining integral, let

$$f(a) = \int_0^\infty \frac{r \ln(1 - a\ sech\ r)}{\sinh\ r \cosh\ r} dr \tag{17}$$

for which $f(1) = X/4\pi^2$ and $f(0) = 0$. By differentiation with respect to a and partial fraction decomposition, we obtain

$$(1-a^2)\frac{df}{da} =$$

$$\int_0^\infty \frac{rdr}{\sinh\ r} - 2a \int_0^\infty \frac{rdr}{\sinh\ 2r} - \frac{1}{a} \int_0^\infty r \sinh\ r \left[\frac{1}{\cosh\ r} - \frac{1}{\cosh\ r + a}\right]. \tag{18}$$

The first two integrals on the right hand side of (18) are tabulated[9] and, after an integration by parts, we find

$$(1-a^2)\frac{df}{da} = \frac{\pi^2}{8}(2-a) - \frac{1}{a}\int_0^\infty \ln(1 + a\ sech\ r) dr \tag{19}$$

The substitution $u = sech\ r$ leads to another tabulated integral[10], giving

$$\frac{df}{da} = -\frac{\pi^2}{8a}\left(\frac{1-a}{1+a}\right) + \frac{1}{2a}\frac{(\cos^{-1} a)^2}{1-a^2}, \tag{20}$$

which, with the substitution $a = \cos\ \theta$ yields

$$X = 4\pi^2 \int_0^1 \frac{df}{da} da = \pi^4 \ln(2) + 4\pi^2 \int_0^{\pi/2} \frac{d\theta}{\sin\ 2\theta}[\theta^2 - \frac{\pi^2}{8}(1 - \cos(2\theta))]. \tag{21}$$

Finally, we find by setting $\phi = 2\theta$, and folding the new range of integration $[\pi/2, \pi]$ back to $[0, \pi/2]$

$$X = \pi^4 \ln(2) + 4\pi^2 \int_0^{\pi/2} \frac{4\phi(\phi - \pi)}{\sin\ \phi} d\phi =$$

$$\pi^4 \ln(2) - \frac{7}{2}\pi^2\zeta(3), \tag{22}$$

where we have used[11]

$$\int_0^{\pi/2} \frac{\phi d\phi}{\sin\ \phi} = 2\mathbf{G}, \qquad \int_0^{\pi/2} \frac{\phi^2 d\phi}{\sin\ \phi} = 2\pi\mathbf{G} - \frac{7}{2}\zeta(3) \tag{23}$$

in which **G** denotes Catalan's constant.

Discussion

Our result is that we have obtained closed form expressions for the two six-fold integrals in (4)

$$X_1 = -\pi^4 \left[\frac{4}{3}\ln(2) - \frac{5}{\pi^2}\zeta(3)\right] = \tag{24}$$

$$-30.7059852392488992576226844460848153687585520816594591898164584 6\ldots$$

$$X_2 = \pi^4 \left[\frac{2}{3}\ln(2) - \frac{2}{\pi^2}\zeta(3)\right] = \tag{25}$$

$$21.2849056705163379834025985474977844006257304408101322209956960 61\ldots$$

This gives the value

$$\Sigma_{2x} = \tag{26}$$

$$0.0241791589181444058954507621628984314049152384251207335945309986\ldots$$

in agreement with Ziesche's [6] seven place calculation. We hope to extend our calculation to an electron gas of arbitrary dimension, as was done for E_{2x}.

Acknowlegements

The first author thanks Dr. Paul Ziesche for a discussion of his work and the National Science foundation for support under Grant DMR 0121146.

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